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From: Arguto, William
Sent: Fri 2/14/2014 4:04:35 PM
Subject: MCHM degradation products

Walt – Thank you for forwarding the information and questions from Dr. Ney regarding MCHM degradation products. Our response, provided below, is the result of discussions from a team of EPA program specialists, laboratory analysts, and research chemists. I have also included Lora Werner, of ATSDR on this response who had also received the request.

Dr. Ney details concerns and suggestions regarding degradation of MCHM and prediction of its properties relevant to its fate, transport, and toxicity.

Before receipt of Dr. Ney's concerns, EPA had been discussing degradation of MCHM and the examination of gas chromatography mass spectrometry (GC/MS) data for potential degradation products. There are a number of highly qualified laboratories involved in response to the Elk River spill. All are using GC/MS to detect and quantify MCHM. GC/MS is a sensitive technique that uses two compound identifiers; chromatographic separation and mass spectral signature. We believe possible MCHM volatile or semivolatile degradation products can be investigated using GC/MS, and we are currently involved in this effort. In response to Dr. Ney's inquiry regarding methods for sample collection and determinative steps: samples are being collected and analyzed in accordance with standard EPA protocols for the analysis of organic compounds in water (e.g., EPA SW846 Methods 3500C, 3510C, and 8270D--available at <http://www.epa.gov/epawaste/hazard/testmethods/sw846/>).

As for predicting properties, relevant fate properties have recently been predicted for MCHM through the use of EPA's EPI Suite™ software (<http://www.epa.gov/oppt/exposure/pubs/episuite.htm>). Description of the fate of MCHM in environmental media now appears in the National Library of Medicine's TOXNET HSDB database. Dr. Ney will notice by the peer review dates shown in the database that this is a recent addition to the database. This information can be accessed by going to <http://toxnet.nlm.nih.gov/>, searching for "4-methylcyclohexane methanol", and then pressing the "HSDB" button to access the report. The TOXNET HSDB database makes use of the same parameters Dr. Ney mentioned to predict the fate.

With regards to the specific degradation products themselves, we are looking at those consistent with the treatment processes utilized at the affected water treatment plant. This is based on the presence of functional groups present in the molecule that are known to react with water treatment chemicals and form by-products. There is a rich history reported in the literature to help understand which functional groups may be reactive. We are also looking at biodegradation products of MCHM and the effect of water treatment chemicals on these, as well. Biodegradation may be a less likely route, but we did not want to discount it.

Dr. Ney recommends exploring the availability of EPA residue data on MCHM to help inform conclusions. In looking up registered pesticides at <http://www.pesticideinfo.org>, we could not

find MCHM registered as a pesticide, so we wouldn't expect EPA to have the type of information about residues required for registered pesticides. We also found that cyclohexanol, which Dr. Ney suggests as a degradation product of MCHM, is also listed as a solvent, not a registered pesticide.

EPA considered Dr. Ney's indication of possible formation of nitrosamine and other nitro compounds from MCHM. It is unclear how cyclohexanol can degrade to nitrophenol in the aqueous environment. This would seem to involve converting a cycloalkane to a cycloaromatic ring, which likely requires much higher temperature, reagents, and special conditions that are different than found in a drinking water plant. Further, to form the nitrophenol, there would need to be a source of nitrogen, and MCHM does not contain nitrogen. If Dr. Ney has any specific scientific literature to share for this synthetic route, we would be interested and would appreciate receiving it. Regardless of whether our level of understanding of cyclohexane chemistry is sufficient, we will note that method 8270D will detect various nitro compounds, including the one Dr. Ney is concerned about. Method 8270D lists applicable analytes, and can be found at the link above.

We also looked into the prediction of toxicity by *Fujitsu CAChe*. We believe that Dr. Ney is referring to *Fujitsu CAChe*, which is software that enables quantitative structure property relationship (QSPR) development, including calculation of molecular mechanical and quantum chemical descriptors. Best we can find, it is currently marketed as "Scigress Explorer" and does not have a built-in capability to predict toxicity, although someone might be able to use the software to develop a suitable QSPR. If Dr. Ney has additional information regarding the development of a suitable QSPR for predicting toxicity, we would be very interested to know this and perhaps speak to the developer.

Regarding the question of radiochemicals present in the water, the consumer confidence report provided by the utility reports its 2011 sampling results for radionuclides, and levels of beta/photon emitters and combined radium are less than the regulated level. We could not develop a reason to believe that the MCHM spill would alter these levels, so please have Dr. Ney forward any additional information or insights regarding radiochemicals relative to MCHM.

Please thank Dr. Ney for forwarding his concerns and suggestions, and we look forward to hearing from you or Dr. Ney if there are any additional concerns and suggestions, or Dr. Ney can send us additional information regarding the points he raised.

Bill Arguto

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